Hysteresis and Dynamic Phase Transition in Kinetic Ising Models and Ultrathin Magnetic Films

Per Arne Rikvold
Florida State University
with many people over many years:
A. Berger, H. Fujisaka, G. Korniss, M. A. Novotny, D. T. Robb,
S. W. Sides, H. Tutu, and C. J. White-Oberlin
http://www.physics.fsu.edu/users/rikvold/info/rikvold.htm
Supported by NSF, DOE, and FSU
Finite-size scaling study of dynamical phase transition in Ising ferromagnet below $T_c$, driven by oscillating field.

Differences from previous finite-size scaling studies of nonequilibrium phase transitions:

- Explicit **time dependence in Hamiltonian**.

- Both “ordered” and “disordered” states **nonstationary** in time and space.

Transition _originally_ observed numerically.
(Lo, Pelcovits, Acharyya, Chakrabarti.)
Ingredients

- **Hysteresis.**
  Results from delayed response in systems subject to periodic applied force.
  - Example: Ferromagnet in oscillating field.

- **Finite-size scaling analysis of critical phenomena.**
  - Major method to analyze numerical data for systems undergoing phase transitions.

- **Decay of metastable phase.**
  Decay of a metastable phase in a spatially extended physical system, driven by thermal nucleation and subsequent growth of droplets.
  - For large systems well described by the Kolmogorov-Johnson-Mehl-Avrami (KJMA) theory.
Model

2D Ising Hamiltonian on $L \times L$ square lattice:

$$\mathcal{H} = -J \sum_{\langle i, j \rangle} s_i s_j - H(t) \sum_i s_i$$

Dimensionless magnetization:

$$m = L^{-2} \sum_i s_i$$

Temperature $T < T_c \Rightarrow m$ for $H=0$ takes one of two degenerate equilibrium values:

$$m(T < T_c, H=0) = \pm m_{eq}(T)$$
Stochastic dynamic

Glauber (nonconserved) dynamic with transition probability

\[ W(s_i \rightarrow -s_i) = \frac{\exp(-\beta \Delta E_i)}{1 + \exp(-\beta \Delta E_i)} \]

where \( \Delta E_i \) is the proposed energy change.
KJMA (Avrami) theory of metastable decay

Following sudden field reversal, critical droplets nucleate at constant rate per unit volume

\[ I(T, H) \propto \exp \left[ -\frac{\Xi(T)}{k_B T H^{d-1}} \right] \]

Large supercritical droplets grow at constant velocity

\[ v \propto |H| \]
Time evolution of magnetization in KJMA theory (randomly placed, freely overlapping droplets):

\[
m(t) \approx m_{eq}(T) \left\{ 2 \exp \left[ -I \int_0^t \Omega_d(vs)^d ds \right] - 1 \right\} \\
= m_{eq}(T) \left\{ 2 \exp \left[ -\frac{\Omega_d}{d+1} \left( \frac{t}{\tau} \right)^{d+1} \right] - 1 \right\}
\]

\[\langle \tau \rangle = (v^d I)^{-\frac{1}{d+1}}\] is average metastable lifetime. \(R_0 \approx \nu \langle \tau \rangle\) is average droplet separation.
Hysteresis

Apply oscillating field,

Commonly: \( H(t) = H_0 \sin(\pi t / t_{1/2}) \)

Or square wave: \( H(t) = H_0(-1)^{\text{int}(t / t_{1/2})} \)

Time-dependent nucleation rate in adiabatic limit:

\[
I(T, H(t)) \propto \exp \left[ - \frac{\Xi(T)}{k_B T H(t)^{d-1}} \right]
\]

and interface velocity

\[
\nu(H(t)) \propto |H(t)|
\]

Scaled field period:

\[
\Theta = \frac{\text{field half-period}}{\text{metastable lifetime}} = \frac{t_{1/2}}{\langle \tau(H_0, T) \rangle}
\]
Symmetry breaking in oscillating field

Ising model in sinusoidal field at $0.8T_c$
Dynamic phase transition
(Square-wave field)

\[ T = 0.8T_c , \ H_0 = 0.3J \]

Low frequency               High frequency

Symmetry breaking!

\[ \frac{H(t)}{H_0} , \ m(t) \]

\[ t \ [\text{MCSS}] \]

Symmetry breaking!
Square-wave Field: Simulation Details

1. Parameters

- Temperature: \( T = 0.8 T_c \)
- Square lattice, \( L = 64, 90, 128, 256, 512 \)
- Applied square-wave field:
  \[
  H(t) = H_0 (-1)^{\text{int}(t/t_{1/2})}, \ H_0 = 0.3 J.
  \]
- Lifetime: \( \langle \tau(H = H_0, T) \rangle = 75 \)
- Droplet separation: \( R_0 \approx 10 \)
- Dimensionless field period: \( \Theta = \frac{t_{1/2}}{\langle \tau(H_0, T) \rangle} \)
- Run lengths: \( 0.3 - 1.5 \times 10^7 \) MCSS

2. Analysis

- Period-averaged magnetization: \( Q = \frac{1}{2 t_{1/2}} \int m(t) dt \)

  is the dynamic order parameter
Dimensionless period: $\Theta = \text{Half-period/Lifetime}$

$T = 0.8T_c, \ H_0 = 0.3J$

Analyze the period-averaged order parameter

$$Q = \frac{1}{2t_{1/2}} \int m(t) \, dt$$
Configurations of local $Q_i$

\[ T = 0.8T_c, \ H_0 = 0.3J, \ L = 128 \]

\[ \Theta = 0.27 < \Theta_c \]
Ordered

\[ \Theta = 0.98 \sim \Theta_c \]
Critical

\[ \Theta = 2.7 > \Theta_c \]
Disordered
Finite-size scaling

Fourth-order cumulant ratio

\[ U_L = 1 - \frac{\langle |Q|^4 \rangle_L}{3 \langle |Q|^2 \rangle_L^2} \]

Describes shape of order-parameter distribution. Fixed point

\[ U^* = 0.611(3), \ \Theta_c = 0.918(5) \]
Order parameter vs $\Theta$

$T = 0.8T_c, H_0 = 0.3J$

Scaling relation: $|Q(\Theta_c)| \sim L^{-\beta/\nu}$

$\beta/\nu = 0.126(5)$

Ising: $\beta/\nu = 0.125$
Scaling plot for $\beta/\nu$

Scaling relation

$$\langle |Q(\Theta_c)| \rangle \propto L^{-\beta/\nu}$$

$\beta/\nu = 0.126(5)$

Ising: $\beta/\nu = 0.125$
Order-parameter fluctuations vs $\Theta$

$T = 0.8 T_c \ , \ H_0 = 0.3J$

Scaling relation at $\Theta_c$: $X = L^{2 \text{Var}(|Q|)} \sim L^{\gamma/\nu}$

$\gamma/\nu = 1.74(5)$

Ising: $\gamma/\nu = 1.75$
Scaling plot for $\gamma/\nu$

$$X = L^2 \text{Var}(|Q|) = L^2 \left[ \langle |Q|^2 \rangle - \langle |Q| \rangle^2 \right] \propto L^{\gamma/\nu}$$

Using fluctuations at $\Theta_c$:

Using fluctuations at maximum

Ising:

$\gamma/\nu = 1.74(5)$

$\gamma/\nu = 1.75$

Ising:

$\gamma/\nu = 1.78(5)$

$\gamma/\nu = 1.75$
Scaling plot for $1/\nu$

$$|\Theta_{\text{max}} - \Theta_c| \propto L^{-1/\nu}$$

yields $\nu = 0.95 \pm 0.15$

Ising: $\nu = 1$
Scaling of order-parameter distribution, $P_L(|Q|)$

Scaling with Ising exponents, $\beta/\nu = 1/8$

Conclusion: This nonequilibrium phase transition is in the equilibrium Ising universality class!!

(Confirmed analytically, Fujisaka, Tutu, Rikvold PRE 63, 036109 (2001))
Experimental observation

$[\text{Co/Pt}]_3$ multilayer under oscillating field with nonzero bias

Experimental multilayer system (A. Berger, D. T. Robb, et al.)

- \([\text{Co}(0.4\text{nm}) \ / \ \text{Pt}(0.7 \text{ nm})]_3\) multilayer. Lateral grain size: 30-300 nm
- **Strong perpendicular anisotropy**
  → Little effect from demagnetizing field
- Apply out-of-plane periodic magnetic field with electromagnet, as well as small constant “bias field” of varying strength
- Measure magnetic field with Hall probe, and magnetization response with **MOKE** (Magneto-Optic Kerr Effect) beam (spot size \(\approx 1 \text{ mm}^2\))
Experimental evidence for DPT: metastable state

- $Q_i$ vs $i$ in experiment at $P = 7.6$ s, in varying bias fields. Similar to $Q_i$ vs $i$ in simulation at $P = 500$ MCSS = 0.95$P_c$ (with comparable bias)

- Metastable dynamically ordered state in weak negative bias field
Evidence for DPT: non-equilibrium phase diagram (NEPD)

\[ \langle Q_i \rangle(P, H_b) \], in analogy with equilibrium phase diagram \[ \langle m \rangle(T, H) \]

- Similarity: large change in \[ \langle Q_i \rangle \] over small range of \[ H_b \] as \[ P \rightarrow P_{c+} \]

- Difference: greater impact of a given bias field for \[ P > P_c \] in experiment (believed to be caused by pinning in reversal process)
In equilibrium Ising system, fluctuations $\sigma_m(T, H)$ increase as $T \to T_c$ and $H \to 0$.

By analogy, near DPT in kinetic Ising simulation, $\sigma_Q(T, H)$ increases as $P \to P_c$ and $H_b \to 0$: similar trend in experiment.
Natural questions about the DPT

1. Given the experimental results, is there a field $H_c$ conjugate to $Q$, analogous to the magnetic field $H$ in the equilibrium Ising model?
   
   **A:** Yes, the period-averaged magnetic field (‘bias field’) $H_b$, as suggested by the recent experiments on [Co/Pt]-multilayers, is the conjugate field $H_c$.

2. In the equilibrium Ising system, a fluctuation-dissipation relation (FDR) holds everywhere. Assuming $H_c$ exists, is there a corresponding FDR between $Q$ and $H_c$?
   
   **A:** Yes, in the critical region (above $P = P_c$), for $H_c$ not too large, an FDR between $Q$ and $H_c$ holds to a very good approximation.

**Definition of** $H_b$, **direct scaling at** $P = P_c$

$$H_b = \int_{t=iP}^{t=(i+1)P} H(t) \, dt$$

defines the period-averaged magnetic field, or ‘bias field’

- find power-law $\langle Q \rangle \sim H_b^{1/\delta'}$ at
  $$P = P_c \text{ with } \delta' = 14.85 \pm 0.18$$
- analogous to equilibrium scaling $\langle m \rangle \sim H^{1/\delta}$ at $T = T_c$, with $\delta = 15$
- note finite-size effects
Predictions from finite-size scaling analysis

- Treat finite-size effects in DPT systematically by writing scaling functions analogous to those used for equilibrium system

  Scaling variables: \( y_1 \equiv \theta L^{1/\nu} \equiv \left( \frac{P - P_c}{P_c} \right) L^{1/\nu} \quad y_2 \equiv H_c L^{\beta\delta/\nu} \)

  Scaling functions: \( \mathcal{F}_+(y_1, y_2) \equiv \langle Q \rangle L^{\beta/\nu} \quad \mathcal{G}_+(y_1, y_2) \equiv \hat{\chi}_L L^{-\gamma/\nu} \)

- Predicted asymptotic forms for scaling functions:

  \[ \mathcal{F}_+(y_1, y_2) \sim \begin{cases} y_1^{-\gamma} y_2 & \text{for } y_1 \gg y_2 \\ y_2^{1/\delta} & \text{for } y_1 \ll y_2 \end{cases} \quad \mathcal{G}_+(y_1, y_2) \sim \begin{cases} y_1^{-\gamma} & \text{for } y_1 \gg y_2 \\ y_2^{(1-\delta)/\delta} & \text{for } y_1 \ll y_2 \end{cases} \]
Numerical results for first scaling function \( (\mathcal{F}_+) \)

- Find \( \mathcal{F}_+ \sim y_1^{-\gamma'} \) with
  \[ \gamma' = -1.76 \pm 0.07 \text{ for } y_1 \gg y_2 \]

- Find \( \mathcal{F}_+ \sim y_2^{\omega'} \) with
  \[ \omega' = 1.01 \pm 0.01 \text{ for } y_1 \gg y_2 \]
Form of nonequilibrium FDR

• Equilibrium FDR: \[
\frac{\partial \langle m \rangle}{\partial H} \equiv \chi_L^M = \frac{L^2 \sigma_M^2}{T} \equiv \frac{X_L^M}{T}
\]

holds for all \((H,T)\), since it follows directly from the partition function

• Nonequilibrium FDR: does it hold?

\[
\frac{\partial \langle Q \rangle}{\partial H_b} \equiv \hat{\chi}_L = \frac{L^2 \sigma_Q^2}{T_{\text{eff}}} \equiv \frac{X_Q^L}{T_{\text{eff}}}
\]
Numerical data on FDR

\[ X^Q_L = T_{\text{eff}} \hat{\chi}_L \]

- For \( P_c < P < 190 \) MCSS, find \( X^Q_L \sim \hat{\chi}_L \) over wide range of \( \hat{\chi}_L \)
  \((P_c = 136.96 \pm 0.75) \text{MCSS}\)

- For \( P \geq 220 \) MCSS, ‘doubly linear’ behavior \( \Rightarrow \) no unique \( T_{\text{eff}} \)
Numerical data on FDR: data at large $H_b$

- At low $\hat{\chi}_L$ values (large $H_b$ values), relation $X^Q_L \sim \hat{\chi}_L$ breaks down.

- Use of $X^Q_L$ as proxy for $\hat{\chi}_L$ in previous work (before $H_b$ was identified) is still well-justified near $P = P_c$. 
$T_{\text{eff}}$ versus $\Theta = (P - P_c)/P_c$
Expected slope: $-\gamma = -1.75$

Expected slope: $(1-\delta)/\delta = -14/15 = -0.933$

Scaling functions $G$ for susceptibility $\chi$ and fluctuation $X$.
Conclusions

- Hysteresis is a far-from-equilibrium phenomenon found in many physical and chemical contexts, including magnetism, ferroelectrics, and surface adsorption.
- Dynamic phase transition (DPT) for kinetic Ising model driven by oscillating field.
- Numerical and analytical evidence shows that the DPT at intermediate frequency is in the equilibrium Ising universality class.
- Experimental evidence for DPT in Pt/Co multilayers.
- Identified bias field as field conjugate to dynamic order parameter.
- Numerically demonstrated nonequilibrium Fluctuation-Dissipation relation in the critical region.